

The logo of the University of Bordeaux is displayed against a background with a blue diagonal stripe in the top left and a dark grey diagonal stripe in the bottom right. The text 'université' is in a dark brown sans-serif font, with the 'u' and 'e' featuring blue highlights. Below it, 'de' is in a smaller dark brown font, and 'BORDEAUX' is in a larger, bold, dark brown sans-serif font.

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Python pour la biologie

Biopython



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BIOINFORMATIQUE

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SeqRecord class from Bio.SeqRecord

- Allows higher level features such as identifiers and features (as SeqFeature objects) to be associated with the sequence, and is used throughout the sequence input/output interface Bio.SeqIO described later.
- Using richly annotated sequence data, say from GenBank or EMBL files,
- Cover most things to do with the SeqRecord and SeqFeature objects
- Read the SeqRecord wiki page (<http://biopython.org/wiki/SeqRecord>), and the built in documentation (also online SeqRecord and SeqFeature)

```
>>> from Bio.SeqRecord import SeqRecord
>>> help(SeqRecord)
...
```

The SeqRecord Object from Bio.SeqRecord module

- `.seq` - The sequence itself, typically a Seqobject.
- `.id` - The primary ID used to identify the sequence – string
 - › (In most cases this is something like an accession number).
- `.name` – A “common” name/id for the sequence – string
 - › (In some cases this will be the same as the accession number, but it could also be a clone name). analogous to the LOCUS id in a GenBank record.
- `.description` - A human readable description or expressive name for the sequence – string
- `.letter_annotations` - Holds per-letter-annotations using a (restricted) dictionary of additional information about the letters in the sequence.

The SeqRecord Object (2)

- `.letter_annotations` - Holds per-letter-annotations using a (restricted) dictionary of additional information about the letters in the sequence.
- `.annotations` - A dictionary of additional information about the sequence. The keys are the name of the information, and the information is contained in the value.
- `.features` - A list of SeqFeature objects with more structured information about the features on a sequence (e.g. position of genes on a genome, or domains on a protein sequence)
- `.dbxrefs` - A list of database cross-references as strings.

Creating a SeqRecord from scratch

- Usually you won't create a SeqRecord “by hand”, but instead use Bio.SeqIO to read in a sequence file for you
- Create a SeqRecord

```
>>> from Bio.Seq import Seq
>>> simple_seq = Seq("GATC")
>>> from Bio.SeqRecord import SeqRecord
>>> simple_seq_r = SeqRecord(simple_seq)
```

- Pass the id, name and description to the initialization function or create later

```
>>> simple_seq_r.id
'<unknown id>'
>>> simple_seq_r.id = "AC12345"
>>> simple_seq_r.description = "Made up sequence I wish I could write a paper about"
>>> print(simple_seq_r.description)
Made up sequence I wish I could write a paper about
>>> simple_seq_r.seq
Seq('GATC', Alphabet())
```

Creating a SeqRecord from scratch(2)

→ Identifier is very important if you want to output your SeqRecord to a file

```
>>> from Bio.Seq import Seq
>>> simple_seq = Seq("GATC")
>>> from Bio.SeqRecord import SeqRecord
>>> simple_seq_r = SeqRecord(simple_seq, id="AC12345")
```

→ The SeqRecord has an dictionary attribute annotations

```
>>> simple_seq_r.annotations["evidence"] = "None. I just made it up."
>>> print(simple_seq_r.annotations)
{'evidence': 'None. I just made it up.'}
>>> print(simple_seq_r.annotations["evidence"])
None. I just made it up.
```

→ Working with per-letter-annotations is similar, letter_annotations is a dictionary like attribute which will let you assign any Python sequence (i.e. a string, list or tuple) which has the same length as the sequence

```
>>> simple_seq_r.letter_annotations["phred_quality"] = [40, 40, 38, 30]
>>> print(simple_seq_r.letter_annotations)
{'phred_quality': [40, 40, 38, 30]}
>>> print(simple_seq_r.letter_annotations["phred_quality"])
[40, 40, 38, 30]
```

SeqRecord objects from FASTA files

→ https://github.com/biopython/biopython/blob/master/Tests/GenBank/NC_005816.fna

```
>gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus ... pPCP1, complete sequence
TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGGGGGTAATCTGCTCTCC
...
```

```
>>> from Bio import SeqIO
>>> record = SeqIO.read("NC_005816.fna", "fasta")
>>> record
SeqRecord(seq=Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG',
SingleLetterAlphabet()), id='gi|45478711|ref|NC_005816.1|', name='gi|45478711|ref|NC_005816.1|',
description='gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus ... sequence',
dbxrefs=[])
```

```
>>> record.seq
Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG', SingleLetterAlphabet())
```


SeqRecord objects from FASTA files (2)

- The first word (after removing the > symbol) is used for both the id and name attributes
- The whole title line (after removing the greater than symbol) is used for the record description

```
>>> record.id
'gi|45478711|ref|NC_005816.1|'
>>> record.name
'gi|45478711|ref|NC_005816.1|'
>>> record.description
'gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus ... pPCP1, complete sequence'
```

- Note that none of the other annotation attributes get populated when reading a FASTA file

```
>>> record.dbxrefs
[]
>>> record.annotations
{}
>>> record.letter_annotations
{}
>>> record.features
[]
```

SeqRecord objects from GenBank files

- https://github.com/biopython/biopython/blob/master/Tests/GenBank/NC_005816.gb
- Contains a single record (i.e. only one LOCUS line) and starts:

```
LOCUS NC_005816 9609 bp DNA circular BCT 21-JUL-2008
DEFINITION Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete
sequence.
ACCESSION NC_005816
VERSION NC_005816.1 GI:45478711
PROJECT GenomeProject:10638
...
```

- Contains a single record (i.e. only one LOCUS line) and starts:

```
>>> from Bio import SeqIO
>>> record = SeqIO.read("NC_005816.gb", "genbank")
>>> record
SeqRecord(seq=Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG',
IUPACAmbiguousDNA()), id='NC_005816.1', name='NC_005816',
description='Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.',
dbxrefs=['Project:10638'])
```

- Automatically assign a more specific alphabet

```
>>> record.seq
Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG', IUPACAmbiguousDNA())
```

SeqRecord objects from GenBank files (2)

- The name comes from the LOCUS line, while the id includes the version suffix. The description comes from the DEFINITION line:

```
>>> record.id
'NC_005816.1'
>>> record.name
'NC_005816'
>>> record.description
'Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.'
```

- GenBank files don't have any per-letter annotations:

```
>>> record.letter_annotations
{}
```

- Most of the annotations information gets recorded in the annotations dictionary, for example:

```
>>> len(record.annotations)
11
>>> record.annotations["source"]
'Yersinia pestis biovar Microtus str. 91001'
```

- The dbxrefs list gets populated from any PROJECT or DBLINK lines:

```
>>> record.dbxrefs
['Project:10638']
>>> len(record.features)
29
```

SeqFeature objects

- Attempts to encapsulate as much of the information about the sequence as possible
- Based on the GenBank/EMBL feature tables
- The key idea about each SeqFeature object is to describe a region on a parent sequence, typically a SeqRecord object
- This region is described with a location object, typically a range between two positions

- **.type** - This is a textual description of the type of feature (for instance, this will be something like `CDS` or `gene`).
- **.location** - The location of the SeqFeature on the sequence that you are dealing with. The SeqFeature delegates much of its functionality to the location object, and includes a number of shortcut attributes for properties of the location:
 - › **.ref** - shorthand for **.location.ref** - any (different) reference sequence the location is referring to (Usually just None).
 - › **.ref_db** - shorthand for **.location.ref_db** - specifies the database any identifier in **.ref** refers to (Usually just None).
 - › **.strand** - shorthand for **.location.strand** - the strand on the sequence that the feature is located on. For double stranded nucleotide sequence this may either be 1 for the top strand, -1 for the bottom strand, 0 if the strand is important but is unknown, or None if it doesn't matter. This is None for proteins, or single stranded sequences.

SeqFeatures functionalities

- **.qualifiers** - Python dictionary of additional information about the feature.
 - › The key is some kind of terse one-word description of what the information contained in the value is about, and the value is the actual information.
 - › For example, a common key for a qualifier might be “evidence” and the value might be “computational (non-experimental).” This is just a way to let the person who is looking at the feature know that it has not been experimentally (i. e. in a wet lab) confirmed.

- **.sub_features** - Represent features with complicated locations like `joins` in GenBank/EMBL files.
 - › This has been deprecated with the introduction of the CompoundLocation object, and should now be ignored.

Positions and locations

→ Position

- › This refers to a single position on a sequence, which may be fuzzy or not. For instance, 5, 20, <100 and >200 are all positions.

→ Location

- › A location is region of sequence bounded by some positions. For instance 5..20 (i. e. 5 to 20) is a location

→ FeatureLocation object

- › Need start and end coordinates and a strand

→ CompoundLocation object

- › Made up of several region

→ FuzzyLocation

- › Several types of fuzzy positions, so we have five classes do deal with them

Fuzzy positions

→ ExactPosition

- › Represents a position which is specified as exact along the sequence. a number, and you can get the position by looking at the position attribute of the object.

→ BeforePosition

- › Represents a fuzzy position that occurs prior to some specified site. In GenBank/EMBL notation, this is represented as something like '<13', signifying that the real position is located somewhere less than 13. To get the specified upper boundary, look at the position attribute of the object.

→ AfterPosition

- › Represents a position that occurs after some specified site. This is represented in GenBank as '>13', and like BeforePosition, you get the boundary number by looking at the position attribute of the object.

Fuzzy positions (2)

→ WithinPosition

- › Models a position which occurs somewhere between two specified nucleotides. In GenBank/EMBL notation, this would be represented as '(1.5)', to represent that the position is somewhere within the range 1 to 5. To get the information in this class you have to look at two attributes. The position attribute specifies the lower boundary of the range we are looking at, so in our example case this would be one. The extension attribute specifies the range to the higher boundary, so in this case it would be 4. So `object.position` is the lower boundary and `object.position + object.extension` is the upper boundary.

→ OneOfPosition

- › Occasionally used for GenBank/EMBL locations, this class deals with a position where several possible values exist, for instance you could use this if the start codon was unclear and there were two candidates for the start of the gene. Alternatively, that might be handled explicitly as two related gene features.

→ UnknownPosition

- › This class deals with a position of unknown location. This is not used in GenBank/EMBL, but corresponds to the '?' feature coordinate used in UniProt.

Fuzzy positions (3)

→ Here's an example where we create a location with fuzzy end points:

```
>>> from Bio import SeqFeature
>>> start_pos = SeqFeature.AfterPosition(5)
>>> end_pos = SeqFeature.BetweenPosition(9, left=8, right=9)
>>> my_location = SeqFeature.FeatureLocation(start_pos, end_pos)
>>> print(my_location)
[>5:(8^9)]
```

- Note that the details of some of the fuzzy-locations changed in Biopython 1.59, in particular for `BetweenPosition` and `WithinPosition` you must now make it explicit which integer position should be used for slicing etc.
- For a start position this is generally the lower (left) value, while for an end position this would generally be the higher (right) value

```
>>> my_location.start
AfterPosition(5)
>>> print(my_location.start)
>5
>>> my_location.end
BetweenPosition(9, left=8, right=9)
>>> print(my_location.end)
(8^9)
```

Fuzzy positions (4)

- If you don't want to deal with fuzzy positions and just want numbers, they are actually subclasses of integers so should work like integers:

```
>>> int(my_location.start)
5
>>> int(my_location.end)
9
```

- For compatibility with older versions of Biopython you can ask for the `nofuzzy_start` and `nofuzzy_end` attributes of the location which are plain integers:

```
>>> my_location.nofuzzy_start
5
>>> my_location.nofuzzy_end
9
```

```
>>> exact_location = SeqFeature.FeatureLocation(5, 9)
>>> print(exact_location)
[5:9]
>>> exact_location.start
ExactPosition(5)
>>> int(exact_location.start)
5
>>> exact_location.nofuzzy_start
5
```

Keyword « in »

- See if the base/residue for a parent coordinate is within the feature/location or not ?

```
>>> from Bio import SeqIO
>>> my_snp = 4350
>>> record = SeqIO.read("NC_005816.gb", "genbank")
>>> for feature in record.features:
... if my_snp in feature:
... print("%s %s" % (feature.type, feature.qualifiers.get('db_xref')))
...
source ['taxon:229193']
gene ['GenelD:2767712']
CDS ['GI:45478716', 'GenelD:2767712']
```

- Note that gene and CDS features from GenBank or EMBL files defined with joins are the union of the exons - they do not cover any introns.

Sequence described by a feature or location

- A SeqFeature or location object doesn't directly contain a sequence
- The location describes how to get this from the parent sequence

```
>>> from Bio.Seq import Seq
>>> from Bio.SeqFeature import SeqFeature, FeatureLocation
>>> example_parent = Seq("ACCGAGACGGCAAAGGCTAGCATAGGTATGAGACTTCCTTCCTGCCAGTGCTGAGGAACTGGGAGCCTAC")
>>> example_feature = SeqFeature(FeatureLocation(5, 18), type="gene", strand=-1)
```

- Take the parent sequence, slice it to extract 5:18, and then take the reverse complement

```
>>> feature_seq = example_parent[example_feature.location.start:example_feature.location.end].reverse_complement()
>>> print(feature_seq) AGCCTTTGCCGTC
```

- SeqFeature object has an extract method to take care of all this

```
>>> feature_seq = example_feature.extract(example_parent)
>>> print(feature_seq)
AGCCTTTGCCGTC
```

- The location describes how to get this from the parent sequence

Sequence described by a feature or location (2)

- The length of a SeqFeature or location matches that of the region of sequence it describes

```
>>> print(example_feature.extract(example_parent))
AGCCTTTGCCGTC
>>> print(len(example_feature.extract(example_parent)))
13
>>> print(len(example_feature))
13
>>> print(len(example_feature.location))
13
```

- For simple FeatureLocation objects the length is just the difference between the start and end positions.
- For a CompoundLocation objects, the length is the sum of the constituent regions

Comparison

→ SeqRecord objects can be very complex, but here's a simple example

```
>>> from Bio.Seq import Seq
>>> from Bio.SeqRecord import SeqRecord
>>> record1 = SeqRecord(Seq("ACGT"), id="test")
>>> record2 = SeqRecord(Seq("ACGT"), id="test")
>>> record1 == record2
```

→ What happens when you try to compare these “identical” records?

→ In older versions of Biopython, `record1 == record2` would only return true if these variables pointed at the same object in memory.

```
>>> record1 == record2
False
```

→ In Biopython 1.67, this will raise an exception

```
>>> record1 == record2
Traceback (most recent call last):
NotImplementedError: SeqRecord comparison is deliberately not implemented. Explicitly compare the attributes of interest.
```

→ you should check the attributes you are interested in

```
>>> record1.id == record2.id
True
>>> record1.seq == record2.seq
True
```

The format method

- Give a string containing your record formatted using one of the output formats supported by Bio.SeqIO, such as FASTA

```
from Bio.Seq import Seq
from Bio.SeqRecord import SeqRecord
from Bio.Alphabet import generic_protein
record = SeqRecord(Seq("MMYQQGCFAGGTVLRLAKDLAENNRGARVLVVCSEITAVTFRGPSETHLDSMVGQALFGD" \
+"GAGAVIVGSDPDLSVERPLYELVWTGATLLPDSEGAIDGHLREVGLTFHLLKDVPGLISK" \
+"NIEKSLKEAFTPLGISDWNSTFWIAHPGGPAILDQVEAKLGLKEEKMRA TREVLSEYGNM" \
+"SSAC", generic_protein),
id="gi|14150838|gb|AAK54648.1|AF376133_1",
description="chalcone synthase [Cucumis sativus]")
print(record.format("fasta"))
>gi|14150838|gb|AAK54648.1|AF376133_1 chalcone synthase [Cucumis sativus]
MMYQQGCFAGGTVLRLAKDLAENNRGARVLVVCSEITAVTFRGPSETHLDSMVGQALFGD
GAGAVIVGSDPDLSVERPLYELVWTGATLLPDSEGAIDGHLREVGLTFHLLKDVPGLISK
NIEKSLKEAFTPLGISDWNSTFWIAHPGGPAILDQVEAKLGLKEEKMRA TREVLSEYGNM
SSAC
```

```
>>> my_location.nofuzzy_start
5
>>> my_location.nofuzzy_end
9
```


Slicing a SeqRecord

- Slice a SeqRecord to give you a new SeqRecord covering just part of the sequence

```
>>> from Bio import SeqIO
>>> record = SeqIO.read("NC_005816.gb", "genbank")
>>> record
SeqRecord(seq=Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG',
IUPACAmbiguousDNA()), id='NC_005816.1', name='NC_005816',
description='Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.',
dbxrefs=['Project:10638'])
>>> len(record)
9609
>>> len(record.features)
41
```

- Any per-letter annotations are also sliced !!
- Any features, completely within the new sequence are preserved (with their locations adjusted).

Slicing a SeqRecord (2)

- Focus in on the pim gene, YP_pPCP05
- In genbank file, gene/CDS has location string [4343..4780]
- In Python counting [4342:4780]

```
>>> print(record.features[20])
type: gene
location: [4342:4780](+)
qualifiers:
  Key: db_xref, Value: ['GeneID:2767712']
  Key: gene, Value: ['pim']
  Key: locus_tag, Value: ['YP_pPCP05']
  <BLANKLINE>
>>> print(record.features[21])
type: CDS
location: [4342:4780](+)
qualifiers:
  Key: codon_start, Value: ['1']
  Key: db_xref, Value: ['GI:45478716', 'GeneID:2767712']
  Key: gene, Value: ['pim']
  Key: locus_tag, Value: ['YP_pPCP05']
  Key: note, Value: ['similar to many previously sequenced pesticin immunity ...']
  Key: product, Value: ['pesticin immunity protein']
  Key: protein_id, Value: ['NP_995571.1']
  Key: transl_table, Value: ['11']
  Key: translation, Value: ['MGGGMISKLFCLALIFLSSSGLAEKNTYTAKDILQNLELNTFGNSLSH...']
```

Slicing a SeqRecord (3)

→ Slice this parent record from 4300 to 4800

```
>>> sub_record = record[4300:4800]
>>> sub_record
SeqRecord(seq=Seq('ATAAATAGATTATTCCAAATAATTTATTTATGTAAGAACAGGATGGGAGGGGGA...TTA',
IUPACAmbiguousDNA()), id='NC_005816.1', name='NC_005816',
description='Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.',
dbxrefs=[])
>>> len(sub_record)
500
>>> len(sub_record.features)
2
```

→ Our sub-record just has two features, the gene and CDS entries for YP_pPCP05:

```
>>> print(sub_record.features[0])
type: gene
location: [42:480](+)
qualifiers:
Key: db_xref, Value: ['GeneID:2767712']
Key: gene, Value: ['pim']
Key: locus_tag, Value: ['YP_pPCP05']
<BLANKLINE>
```

Slicing a SeqRecord (3)

```
>>> print(sub_record.features[1])
type: CDS
location: [42:480](+)
qualifiers:
Key: codon_start, Value: ['1']
Key: db_xref, Value: ['GI:45478716', 'GeneID:2767712']
Key: gene, Value: ['pim']
Key: locus_tag, Value: ['YP_pPCP05']
Key: note, Value: ['similar to many previously sequenced pesticin immunity ...']
Key: product, Value: ['pesticin immunity protein']
Key: protein_id, Value: ['NP_995571.1']
Key: transl_table, Value: ['11']
Key: translation, Value: ['MGGGMISKLFCLALIFLSSSGLAEKNTYTAKDILQNLELNTFGNSLSH...']
```

→ Locations have been adjusted to reflect the new parent sequence!

```
>>> sub_record.annotations
{}
>>> sub_record.dbxrefs
[]
```

Annotations and dbxrefs are omitted from the sub-record !!

```
>>> sub_record.id
'NC_005816.1'
>>> sub_record.name
'NC_005816'
>>> sub_record.description
'Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.'
```

Record id, name and description are preserved !!

Adding SeqRecord objects

- Add SeqRecord objects together, giving a new SeqRecord
- Any common per-letter annotations are also added
- All the features are preserved (with their locations adjusted)
- Any other common annotation is also kept (like the id, name and description)

```
>>> from Bio import SeqIO
>>> record = next(SeqIO.parse("example.fastq", "fastq"))
>>> len(record)
25
>>> print(record.seq)
CCCTTCTTGTCTTCAGCGTTTCTCC
>>> print(record.letter_annotations["phred_quality"])
[26, 26, 18, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 22, 26, 26, 26, 26,
26, 26, 26, 23, 23]
```

```
>>> int(my_location.start)
5
>>> int(my_location.end)
9
```

Adding SeqRecord objects (2)

→ Suppose this was Roche 454 data and think the TTT should be only TT

```
>>> left = record[:20]
>>> print(left.seq)
CCCTTCTTGTCTTCAGCGTT
>>> print(left.letter_annotations["phred_quality"])
[26, 26, 18, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 22, 26, 26, 26]
>>> right = record[21:]
>>> print(right.seq)
CTCC
>>> print(right.letter_annotations["phred_quality"])
[26, 26, 23, 23]
```

→ Now add the two parts together

```
>>> edited = left + right
>>> len(edited)
24
>>> print(edited.seq)
CCCTTCTTGTCTTCAGCGTTCTCC
>>> print(edited.letter_annotations["phred_quality"])
[26, 26, 18, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 22, 26, 26, 26, 26, 26, 26, 23, 23]
```

→ You can make this shorter

```
>>> edited = record[:20] + record[21:]
```

Adding SeqRecord objects (3) –circular genome

```
>>> from Bio import SeqIO
>>> record = SeqIO.read("NC_005816.gb", "genbank")
>>> record
SeqRecord(seq=Seq('TGTAACGAACGGTGAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG',
IUPACAmbiguousDNA()), id='NC_005816.1', name='NC_005816',
description='Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.',
dbxrefs=['Project:10638'])
>>> len(record)
9609
>>> len(record.features)
41
>>> record.dbxrefs
['Project:58037']
>>> record.annotations.keys()
['comment', 'sequence_version', 'source', 'taxonomy', 'keywords', 'references',
'accessions', 'data_file_division', 'date', 'organism', 'gi']
```

→ Shift the origin like this:

```
>>> shifted = record[2000:] + record[:2000]
>>> shifted
SeqRecord(seq=Seq('GATACGCAGTCATATTTTTTACACAATTCTCTAATCCCGACAAGGTCGTAGGTC...GGA',
IUPACAmbiguousDNA()), id='NC_005816.1', name='NC_005816',
description='Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.',
dbxrefs=[])
>>> len(shifted)
9609
```